Lawrence Livermore National Laboratory Proposal to Participate in the Carbon and Metal Hydride Virtual Centers

Robert Glass
LLNL Hydrogen Program Manager

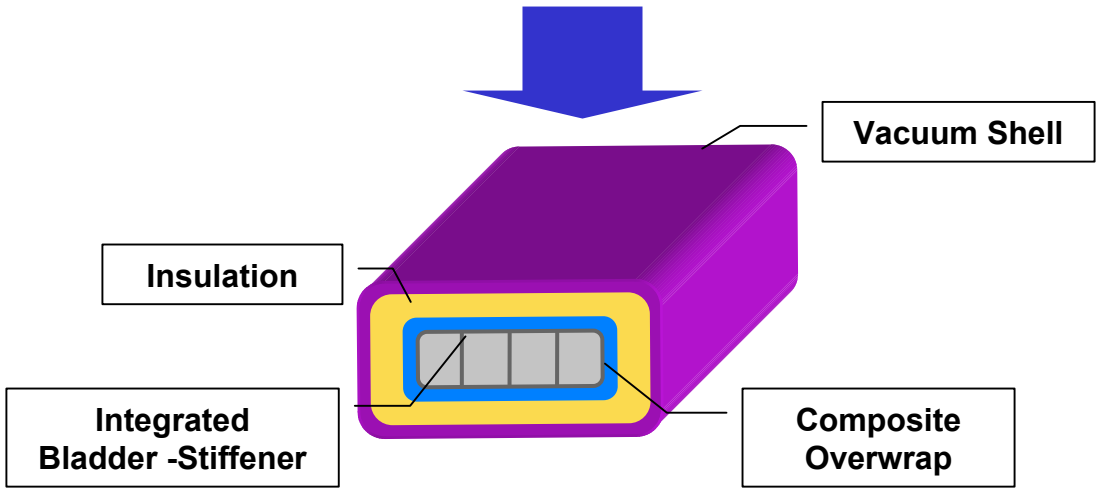
June 19, 2003

LLNL leads the DOE effort in tank R&D

Insulated pressure vessels

Lightweight tanks

- ✓ We have already demonstrated >11% by weight storage
- ✓ Tanks are the “ace in the hole” storage technology

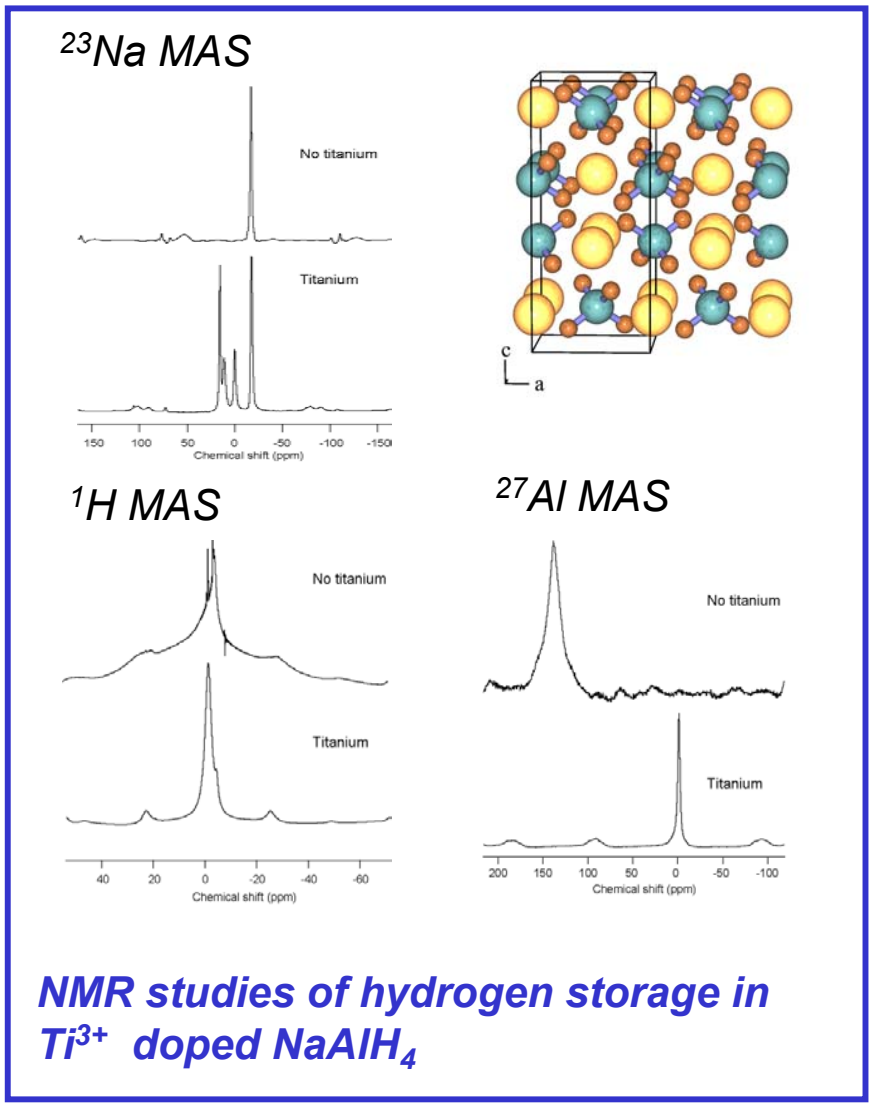


Next generation cryogenic conformable tanks will meet all future storage goals

LLNL has outstanding capability to contribute in several areas of metal hydride and carbon structure hydrogen storage

- ✓ **Molecular dynamics simulation for fundamental understanding of storage mechanisms and properties**
- ✓ **Analytical techniques (solid state NMR, XPS, EXAFS, ESR) to elucidate chemical structures**
- ✓ **We are the premier laboratory in carbon aerogels and have explored their use for hydrogen storage and gas separation**
- ✓ **Other materials technologies (e.g., magnetron sputter deposition) potentially useful for creating high storage capacity structures**

We are using NMR to examine the structure and dynamics of metal hydride H_2 storage systems



NMR studies of hydrogen storage in Ti^{3+} doped $NaAlH_4$

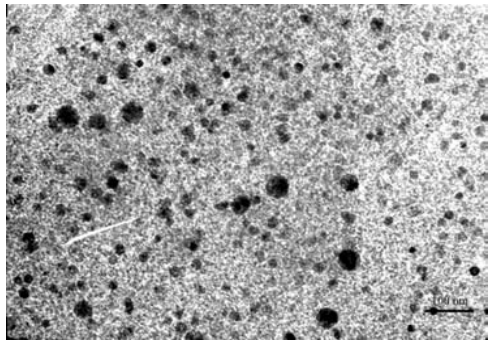
NMR can provide detailed understanding of

- **Structural influence of metal incorporation**
- **Hydrogen speciation**
- **Mode of hydrogen interaction (chemi- or physisorbed)**
- **Release/reversibility mechanisms**

We are studying H_2 storage and the effect of metal doping in $NaAlH_4$ with SNL collaborators. Preliminary studies have been done on carbon aerogel systems.

LLNL new project proposal: Metal-containing organic aerogels for H_2 storage

Concept



TEM of metal nanocrystals in hybrid metal-carbon aerogel

Background

Current carbon and metal hydride systems have not been shown to meet storage goals. New systems are needed. In our work, the technical issues will be: (1) choice of optimum metal(s); (2) optimum carbonization conditions; (3) optimum density for weight and strength; and (4) ultimate storage conditions.

Proposed Technical Approach

We will explore metal-containing organic (carbon) aerogels for hydrogen storage. These materials have intrinsic high storage capacity with active carbon nanostructure and additional capacity due to metal-hydrogen interactions. Our approach uses sol gel techniques to create a structure having repeat units. Each repeat unit has a metal binding site, ensuring uniform dispersion of metal dopant upon ion exchange. A provisional patent has been filed.

Project Goals

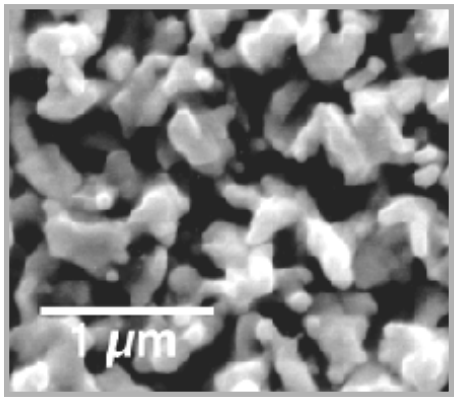
(1) Synthesize light weight and strong materials for H_2 storage
(2) Measure H_2 adsorption/desorption capacities and kinetics
(3) Determine reversibility and material lifetime
(4) Make storage system hardware recommendations

Key Deliverable: Light weight and strong H_2 storage material in a container ready to use

PI: John Reynolds, Lawrence Livermore National Laboratory, (925) 422-6028, reynolds3@llnl.gov

LLNL new project proposal: "Metallic" sponges for hydrogen storage

Concept



An example of a "metallic" sponge deposited using planar magnetron sputtering

A Jankowski, J. Vac. Sci. Technol. A, 21 (2003) 422

Background

Current metal hydride systems do not meet H_2 storage capacity goals, nor do they have acceptable kinetics at lower temperatures for H_2 uptake and release. New approaches are needed to meet these and more demanding goals. Advanced materials engineering of "metallic" sponges offer one potential solution.

Proposed Technical Approach

We will assess the use of vapor-deposits as sponges with controlled pore size for rapid hydrogen storage and release. By maximizing the surface area-to-mass ratio we can exploit the kinetics of surface vs. bulk reactions in reversible hydride systems. We will first demonstrate a metallic-hydride sponge as a thick and porous vapor deposit using a known bulk material (e.g., based on Mg (Ni) or NaAl).

Project Goals

(1) Demonstrate we can deposit a metallic-hydride sponge

(2) Demonstrate improved hydrogen storage capacity using high surface area metallic sponge versus bulk form

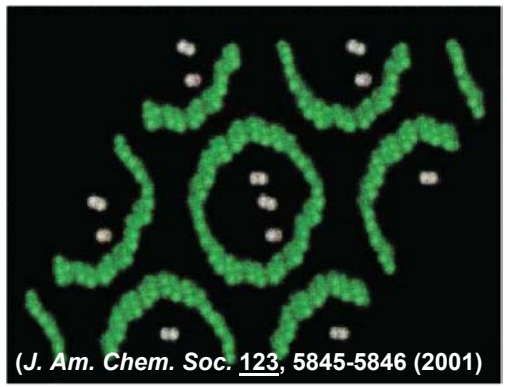
(3) Demonstrate reversible hydrogen storage in multiple cycles, at 6 wt. % or more from multi-cell planar module

<u>Key Deliverable</u>: Multi-cell module for hydrogen storage based on planar components of metallic sponges with >6 wt. % reversible hydrogen storage

PI: Alan Jankowski, Lawrence Livermore National Laboratory, (925) 423-2519, jankowski1@llnl.gov

LLNL new project proposal: Ab initio molecular dynamics simulation of hydrogen storage in carbon nanostructures

Concept



***Ab initio* molecular dynamics simulations of hydrogen in carbon nanotubes**

Background

The mechanism of hydrogen storage in carbon nanotubes is unexplained. Unknowns include the effect of geometry of nanotubes (e.g., diameter, tube ends, orientation of tubes, and the effect of contaminants). *Ab initio* simulations can be used to obtain mechanistic information providing insight into whether nanotubes are H_2 storage systems capable of meeting program goals greater than or equal to 6 wt. %.

Proposed Technical Approach

The objective of this work is to answer key questions concerning the mechanism of hydrogen storage in carbon nanostructures. Our approach will be to use *ab initio* molecular dynamics based on the Car-Parrinello approach with LLNL's newly acquired 11 teraflop MCR parallel computer to compute critical properties concerning storage in carbon nanotubes. This approach will allow molecular dynamics calculations with accuracy and number of atoms not previously possible.

Project Goals

(1) Predict enthalpy of adsorption for single and multiple hydrogens
(2) Determine effect of tube diameter on hydrogen storage
(3) Determine the effect of including metals (e.g., Ti) in the nanostructure

Key Deliverable: Report optimum criteria for hydrogen storage on nanostructures determined from CPMD code calculations

PI: Christopher Mundy, Lawrence Livermore National Laboratory, (925) 422-9571, mundy2@llnl.gov